Development and Application of an Inverse Spatially Offset Raman Spectroscopic Method for the Detection of Concealed Substances

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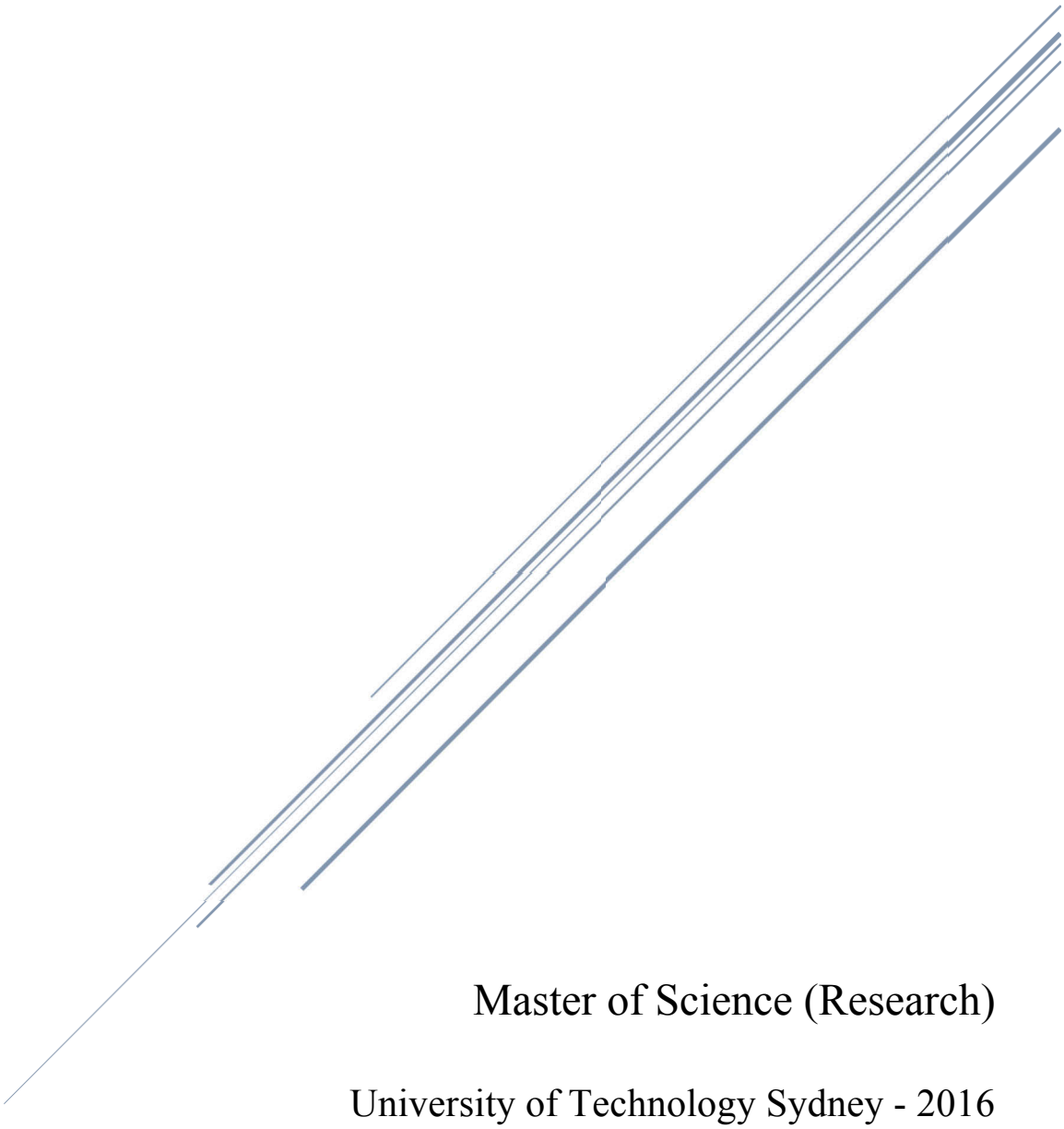

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Abbreviations

AFP	Australian Federal Police
ALS	Alternating Least Squares
API	Active Pharmaceutical Ingredient
BTEM	Band-Target Entropy Minimisation
CCD	Charge Couple Device
DEA	Drug Enforcement Administration
FBI	Federal Bureau of Investigation
HCl	Hydrochloride
HDPE	High Density Polyethylene
GSM	Grams per Square Metre
LDPE	Low Density Polyethylene
LOD	Limit of Detection
LOQ	Limit of Quantification
MCR	Multivariate Curve Resolution
MDMA	3,4-Methylenedioxymethamphetamine (Ecstasy)
NA	Numerical Aperture
NIR	Near Infrared
NIPALS	Non-linear Iterative Partial Least Squares
PARAFAC	Parallel Factor Analysis
PCA	Principal Component Analysis
PED	Performance Enhancing Drug
PLS	Partial Least Squares

PLS-R	Partial Least Squares Regression
PVC	Polyvinyl Chloride
PMMA	Poly(methyl methacrylate)
RMSE	Root Mean Square Error
RMSEP	Root Mean Square Error of Prediction
S	Slope
SD	Standard Deviation
SESORS	Surface Enhanced Spatially Offset Raman Spectroscopy
SNR	Signal to Noise Ratio
SNV	Standard Normal Variate
SORS	Spatially Offset Raman Spectroscopy
UNODC	United Nations Office on Drugs & Crime
WCO	World Customs Organisation
WHO	World Health Organisation

Abstract

Since the creation of the 'Dark Net' in mid-1990's, the way in which drugs are bought, sold, and transported has changed dramatically (Bartlett 2014). A digital age of drug trade has begun, and it has only been growing, with tens of thousands of websites now available on the Darknet, many of which are dedicated to the sale and trade of illicit substances (Anderson 2015). While techniques utilised by Customs and Border Security offices, both domestically and internationally, have evolved to stem this growing problem, the methodologies used by drug transporters and vendors have advanced even more rapidly, causing there to be a growing need for new detection techniques.

In 2016, the postal system has become one of the largest channels through which illicit substances are trafficked, with suppliers simply mailing their products to customers, greatly reducing and even removing the risk of ever being caught. Furthermore, suppliers have adopted a new, 'scatter-gun' approach, in which large shipments are broken down and sent in smaller, less obvious quantities. This approach has two main benefits, firstly, shipments are easier and cheaper to transport, and secondly, if one or two smaller parcels are intercepted, the bulk of the shipment is still far more likely to slip by Customs and Border Security offices. It is the combination of these practises, as well as the inability to examine every piece of mail that is sent and received that has helped to create a growing problem and a damaging trend.

In this paper, a Spatially Offset Raman Spectroscopy (SORS) method was developed and implemented specifically to detect, identify, and quantify samples of illicit substances concealed within twenty-five common packaging types. Utilising an axicon, conventional Raman

spectrometer and chemometric software, it was shown that a rapid and non-destructive SORS method could be easily and successfully implemented for the bulk of packaging materials commonly encountered within Australia and at Australian borders, as well as potentially aiding in the detection and identification of many concealed drug samples.

Ultimately, it was found that nineteen of the twenty-five packaging types could be successfully interrogated using the developed method, with strong signals and accurate detections made through envelopes, padded bags, and a variety of tapes, plastics, and papers. Furthermore, it was found that the method could detect and identify complex, powdered samples involving up to four components, as well as detecting target substances through more complex multi-layered parcels with a relatively high degree of accuracy and certainty.